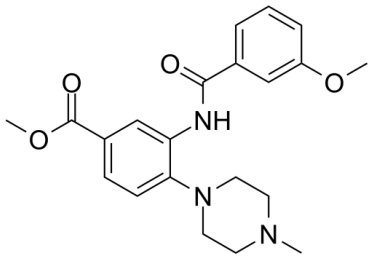
Data Sheet

Product Name:	WDR5-0103
Cat. No.:	CS-5228
CAS No.:	890190-22-4
Molecular Formula:	C21H25N3O4
Molecular Weight:	383.44
Target:	Histone Methyltransferase
Pathway:	Epigenetics
Solubility:	DMSO : ≥ 40 mg/mL (104.32 mM)



BIOLOGICAL ACTIVITY:

WDR5-0103 is a potent and selective WD repeat-containing protein 5 (WDR5) antagonist with Kd of 450 nM. IC50 value: 450 nM (Kd) Target: WDR5 in vitro: WDR5-0103 inhibits MLL catalytic activity with an IC50 value of 39±10 μM. An increase in MLL complex concentration resulted in proportional increase in IC50 values for WDR5-0103 (83±10 and 280±12 μM at concentrations of 500 and 1000 nM of the core trimeric MLL complex respectively). These data are consistent with a mechanism of action in which WDR5-0103 antagonizes the interaction of WDR5 with MLL by competing with MLL for their mutual binding site on WDR5.

PROTOCOL (Extracted from published papers and Only for reference)

Enzyme assay [1] The effect of WDR5-0103 on the activity of the MLL complex was tested in at least duplicate at three different concentrations of trimeric (125, 500 and 1000 nM) and tetrameric (10, 50 and 125 nM) MLL complex. Reactions were carried out in 20 μl of 20 mM Tris/HCl (pH 8.0), 5 mM DTT (dithiothreitol) and 0.01% Triton X-100 in the presence of 2 μM [3H]SAM (S-adenosylmethionine) and 5 μM of biotinylated H3 (1-25) peptide. For IC50 determinations, reaction mixtures with various concentrations of WDR5-0103 (1 μM-1 mM) were incubated for 1 h at room temperature and then quenched by adding 20 μl of 7.5 M guanidinium chloride, followed by the addition of 180 μl of buffer (20 mM Tris/HCl, pH 8.0). The reactions were mixed and transferred to a streptavidin-coated 96-well microplate. The FlashPlates were incubated for at least 1 h and the c.p.m. values were determined using a Topcount plate reader. The IC50 values were determined using SigmaPlot software.

References:

[1]. Senisterra G, et al. Small-molecule inhibition of MLL activity by disruption of its interaction with WDR5. Biochem J. 2013 Jan 1;449(1):151-159.

CAIndexNames:

Benzoic acid, 3-[(3-methoxybenzoyl)amino]-4-(4-methyl-1-piperazinyl)-, methyl ester

SMILES:

O=C(OC)C1=CC=C(N2CCN(C)CC2)C(NC(C3=CC=CC(OC)=C3)=O)=C1

Caution: Product has not been fully validated for medical applications. For research use only.

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